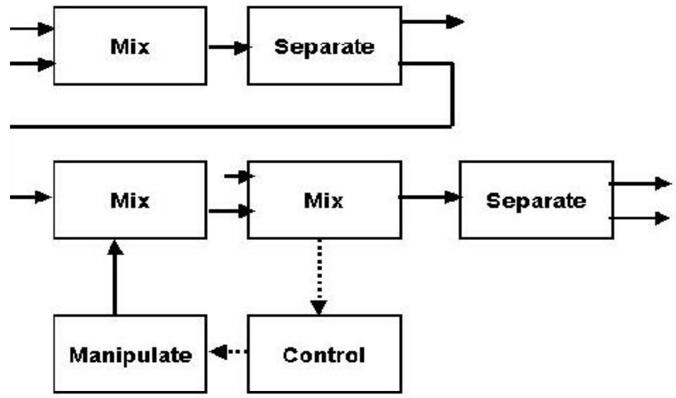
Environmental Simulation Program (ESP)

The Challenge



Saltcake dissolution from a Single Shell Tank depicted as an ESP Flow Diagram

The Hanford Site tank waste system includes diverse inorganic species dissolved in or precipitated from highly concentrated alkaline nitrate brines. The River Protection Project (RPP) must retrieve the waste from these tanks and process it into a final waste form for storage and/or disposal. The ability to treat the waste depends crucially on waste composition, which depends on chemical equilibria and chemical reactions in the tanks. The reactions occur as liquids and solid phases are separated physically, diluted, and mixed during transfers en route to treatment. For each delivery of waste feed to the vitrification plant for the first phase of retrieval and treatment, the RPP must define a process flowsheet to describe the baseline, including a mass balance over all significant species during the transfers, and also define the waste retrieval operations.

Hanford waste is in contact, and often saturated with, numerous salts and metal hydroxides in the solid phase. Dominant components include sodium nitrate, sodium nitrite, sodium carbonate, sodium hydroxide, sodium phosphate, sodium sulfate, and sodium fluoride. Ionic strengths over 20 molal are common. Within this chemical environment, one must be able to predict the disposition of chemically minor but radiologically dominant elements. These include radiologically important elements such as cesium, strontium, and technetium. They also include certain non-radioactive elements, such as chromium, which affect waste treatment processes inordinately compared to their concentrations. Because the liquid phase of Hanford wastes is so concentrated, binary, ternary, and even quaternary interactions among ions must be considered in order to predict the chemical equilibria and subsequent disposition of species of these wastes using thermodynamic models.

Current Approach

Process flowsheets previously developed and quantified at Hanford used chemical simulators that did not adequately describe the chemical equilibria or mass balances among the cations and anions of electrolytes, which constitute essentially all of the liquid phase of Hanford tank waste. Therefore, effective "splits" of species between phases and during dilution had to be determined through expensive experiments. Because the wastes and their

BENEFITS AND FEATURES

- Describes chemical equilibria and resulting mass balances for electrolyte systems
- Standardizes waste chemistry analyses across the site
- Automates much of the development of waste processing flowsheets
- Saves over $2,000,000 per year in technical labor

chemical behavior are so complex, the accuracy of flowsheets and calculations used to define waste retrieval operations were open to question.

New Technology

The Environmental Simulation Program (ESP) is a chemical process flowsheet simulator designed to accurately describe equilibria and consequent process splits among electrolytes. Moreover, the vendor, OLI Systems, Inc., has worked with Hanford contractors to add to the ESP database a number of species important to describing Hanford tank waste, using both the Bromley and Pitzer thermodynamic formulations. Through support of the Tanks Focus Area of the Department of Energy's Environmental Management's Office of Science and Technology, a number of ion association parameters important to describing Hanford tank waste behavior has been added to or improved in the ESP thermodynamic database.

The ESP model is adopted as the standard aqueous process simulator at the Hanford Site. ESP and its predecessor software have been used for over eight years. Simulations evaluate in-tank processing and develop waste feed delivery strategies. ESP is also used for simulating Plutonium Finishing Plant processing options. Since its introduction at the Hanford site, ESP has been used to:

- predict what has leaked from tanks,
- predict the amount of leaching and precipitation from different in-tank sludge washing options,
- examine existing transfer line plugs for determination of what happened and make process changes,
- show ammonia was the cause of a pH decline during tank storage, which was a safety and corrosion issue, and
- identify potential gel formations within alternative waste treatment plant feed streams.

ESP's principal applications at Hanford include developing process flowsheets for RPP, predicting the behavior of concentrated wastes during retrieval operations, and solving problems involving waste precipitation and dissolution. ESP reduces costs caused by over-design and reduces the expensive experimental work needed to obtain the design data. Experimental work requires staff and facilities for radioactive work, adding up to potential avoided costs of over two million dollars per year.

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